

Numerical Simulation of High-Pressure Combustion using Conditional Source-term Estimation

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The applicability of Conditional Source-term Estimation (CSE) for high-pressure combustion applications is investigated within the context of Reynolds Averaged Navier-Stokes equations (RANS). The tabulation of the conditional chemical source-terms, typically done using a trajectory generated low-dimensional manifold, presents a more constrained region of physical realizability, which imposes new constraints on the tabulation. Various approaches are presented and discussed. The applicability of CSE is then tested on a high-pressure methane-oxidizer combustor.

1. Introduction

An increasing number of propulsion devices are operating at high-pressure (high-p) conditions in order to improve their thermodynamic efficiency. Much of the interest in high-p propulsion systems is the result of recent advances in high-temperature/high-pressure resistant materials enabling new opportunities to improve thermodynamic efficiencies. In modern diesel engines, gas turbines, and liquid rocket engines, the combustion occurs at near-critical or at supercritical pressures. Under these extreme thermodynamic conditions, the mixing and combustion differ greatly compared to their low-pressure counterparts. For example, the mixing between the fuel and oxidizer is diffusion dominated while the densities of both streams can resemble that of a liquid. Furthermore, at these pressures, a clear delineation between the gas and liquid phases, as observed in many low-p injection systems, is blurred as both the surface tension and enthalpy of vaporization become null above the critical point. The thermo-physical complexities associated with high-p combustion presents substantial challenges for predictive turbulent combustion simulations which have not yet been fully addressed. A summary of these challenges can be found in the review articles by Bellan [1] and Candel *et al.* [2].

The thermodynamic non-idealities and transport anomalies in high-pressure combustion present significant challenges to existing combustion models. Turbulence-chemistry interaction remains one of the most important – yet often overlooked – aspects of numerical turbulent combustion. The small-scale turbulent fluctuations drive many of the physical processes in non-premixed flames: local straining of the flame, wrinkling of the

flame sheet, and local thermodynamic transport. For most engineering-relevant simulations, and especially in liquid rocket combustion, the large scale-separation means that some level of modeling must be used. Typically, the modeling approaches rest on spatial filtering (in the case of LES) or time-averaging (RANS/URANS) to obtain local thermodynamic and source-term estimates. In case of strong-nonlinear processes, the source-term can no longer be estimated using the averaged or filtered thermodynamic and compositional quantities. In other words:

$$\overline{\dot{\omega}_k} \neq \dot{\omega}_k(\overline{\rho}, \overline{T}, \overline{Y_i}). \quad (1.1)$$

Although a similar closure problem is observed in low-p combustion, the challenges for high-p conditions remains substantial.

Efforts to address the challenges in high-p combustion have been made over the past two decades. Oefelein and Yang [3] are widely recognized as the authors of one of the very first benchmark-quality simulation of supercritical combustion. In the wake of this initial work, efforts have been made to transpose low-p advance in combustion modeling into the supercritical realm. Cutrone *et al.* [4] extended the flamelet-progress-variable approach (FPVA) with a presumed beta Probability Distribution Function (PDF) for the simulation of high-pressure combustion in a Reynolds-Averaged Navier-Stokes (RANS) context. A follow-up contribution investigated the joint PDF modelling for the mixture fraction and progress variable [5]. The applicability of the flamelet assumptions in supercritical combustion was questioned by Zong, Ribert and Yang [6]. They noted that the characteristic length of Kolmogorov scale reduces (through a modification of the thermophysical properties) more rapidly than the characteristic flame thickness; eventually, this may invalidate some of the basic tenets of the flamelet assumption. Other works, such as [7, 8], rely on the dynamic thickened flame approach for non-premixed combustion to account for the turbulent-chemistry interaction. This approach, which is based on a judicious modification of the temporal and spatial scales of combustion (see e.g. [9]), is not universally applicable to all combustion regimes. Other approaches such as linear-eddy model [10] and direct closure [11] approaches have also been proposed.

The shortcoming of all the above-mentioned turbulence-chemistry closure models opens the door to new ideas for high-p combustion. In the present work, we investigate the use of Conditional Source-term Estimation (CSE), which is a computationally efficient variation of the Conditional Moment Closure (CMC) model, for use in high-pressure, non-premixed combustion. The theoretical basis for CSE is presented in section 2. The Trajectory Generated Low-Dimensional Manifold (TGLDM), used to tabulate the chemical source-terms in conditional space, is described in section 3. Finally, exploratory simulations of high-p CSE are presented in section 4.

2. Conditional Source-term estimation

Bushe and Steiner [12] developed the Conditional Source-term Estimation (CSE) method as a computationally advantageous extension to the Conditional Moment Closure (CMC) method. Both approaches stem from the observation that the fluctuations in the reactive species are correlated with a conditioning variable ζ — such as mixture fraction in non-premixed combustion — and the quantities have a much smaller variation about the conditional mean than in physical space. Therefore, the assumption

$$\overline{\dot{\omega}_k | \zeta} \approx \dot{\omega}_k(\overline{\rho | \zeta}, \overline{T | \zeta}, \overline{Y_i | \zeta}) \quad (2.1)$$

can be made about the conditional mean value of the reaction rate $\dot{\omega}_k$. How one gets the conditional averages of the reactive scalars is what differentiates CSE from CMC.

In CMC [13] the transport equations for conditional averages of the reactive scalars are derived and solved. Models are required for many unclosed terms — for the most part, the terms are simply neglected — however, the closure for the chemical source-term is found to be very accurate, provided the conditioning variable (or variables) are chosen well. In non-premixed combustion, if the mixture fraction is used as the conditioning variable and the flame does not exhibit ignition or local extinction, the CMC chemical closure works very well. CMC does not work well for premixed combustion because closure for some of the unclosed terms in the transport equations for the conditional averages is critically important and very difficult to accomplish. CMC also has the drawback that the conditioning variable is added to the system of equations as a new independent variable, so, for flows in relatively complex geometries where the flow would be three dimensional, one must modify the solver to solve in (effectively) four dimensions.

Conditional source-term estimation originated from the desire to use CMC in LES. It has been applied to a number of combustion studies, primarily at atmospheric pressure. Recent works have shown the applicability for study of MILD combustion [14] and partially premixed combustion in lifted flames [15]. CSE has also been successfully extended to account for SGS terms in LES [16].

Rather than solving transport equations for conditional averages, in CSE integral equations are solved within ensembles of points in which the conditional averages are assumed to be homogeneous to obtain approximations of the conditional averages from unconditional averages. Hence, for each point x within ensemble A , one assumes that the conditional average of the reactive scalar f can be well represented by the ensemble average of the conditional averages for all points within that ensemble:

$$\overline{f|\zeta}(\mathbf{x}, t) \approx \langle \overline{f|\zeta} \rangle(t; \mathbf{A}). \quad (2.2)$$

and then solve for that conditional average within the ensemble by inverting this integral equation:

$$\overline{f}(\mathbf{x}, t) \approx \int_0^1 \langle \overline{f|\zeta} \rangle(t; \mathbf{A}) \mathbf{P}(\mathbf{x}, t; \zeta) d\zeta, \quad (2.3)$$

where $P(\mathbf{x}, t; \zeta)$ is the local probability density function (PDF) of the conditioning variable at point \mathbf{x} in the ensemble. The local PDF is usually modeled by a function of the local mean and variance of the conditioning variable.

When CSE is coupled with a low-dimensional manifold chemistry model (which is described in section 3), two reactive scalars $Y_{\text{H}_2\text{O}}$ and Y_{CO_2} are fully transported in physical space and by inverting Eq. 2.3 for the conditioned variable, all mean conditional chemical source terms and conditional species mass fractions can be obtained from the chemistry table W_α that describes the manifold. Fig. 1 is an illustration of the overall process of CSE.

The looked-up values are then plugged into Eq. 2.3 in a forward manner to obtain the unconditional mean reaction rates $\dot{\omega}_k$ and the mean species mass fractions \bar{Y}_k of other species. More details on this approach can be found in [12, 14, 15, 17].

The method provides closure for the chemical source terms of similar fidelity to CMC, however, since transport equations for the conditional averages do not need to be solved, it leads to a dramatically lower-cost (in terms of computational cost) simula-

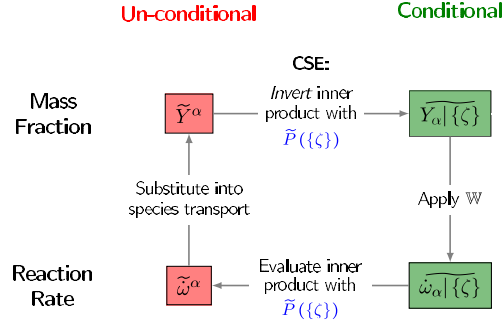


FIGURE 1. CSE procedure - exchange between conditional and unconditional space

tion. The method has already been shown to provide good predictions of non-premixed flames when implemented in Large-Eddy Simulation (LES) [18–20] and in combination Reynolds-Averaged Navier-Stokes (RANS) models [21–23]. It has also been adapted for use in premixed turbulent combustion [24]. Because the premixed and non-premixed models make consistent assumptions, they can be combined to make it possible to address partially premixed combustion problems [25], a method that has come to be known as Doubly-Conditional Source-term Estimation (DCSE). It is also worth noting that the model is identical when implemented in either the RANS or LES paradigm, such that the module coded to implement it does not need to even be informed of which turbulence modeling approach is being used.

When inverting an integral equation, one typically finds it necessary to provide regularization to obtain a physically meaningful solution. For the most part, the simple Tikhonov regularization has proven to work very well in finding the conditional average for the reactive scalars. In zeroth order Tikhonov regularization, one simultaneously tries to find the solution that best matches the provided input while also fitting a linear function, such that one solves this minimization problem for $\langle f|\zeta \rangle$:

$$\min \left\{ \left| M_{jk} \langle f|\zeta \rangle - \bar{f}_j \right| + \lambda \left| \langle f|\zeta \rangle - f_0(\zeta) \right| \right\},$$

where the matrix M_{jk} represents the numerical quadrature of the integral in Eq. 2.3, $f_0(\zeta)$ is the linear function. The constant λ can be arbitrary, however there are rigorous ways of determining an optimal value [26]. Most CSE implementations have used as the input function either a laminar flame or else the solution for the conditional average from the last time step or iteration; this means that CSE is actually calculating how different the conditional average in the given field is from a laminar flame (when we use the laminar flame solution) or how much the conditional average for the field has changed from the last time step or iteration. Other options have become available such as regularizing to a constant or to flat. This gives opportunities to experiment with the initialization of the combustion in a simulation.

As mentioned earlier, every implementation of CSE requires a chemical kinetic mechanism and a model for the PDF of the conditioning variable. Due to the nature of this method there exists a high dependency on the accuracy of the PDF as it is used twice in the process to transition between conditional and unconditional variables. To our knowledge, this approach has yet to find its way into high-speed, high-pressure combustion, mostly due to a lack of reliable direct numerical simulations data, which is necessary to validate the use of certain PDFs. Recent work by Bellan [27] investigated a number

of assumptions underpinning CSE and noted the lack of accuracy of the β -PDF in the high-pressure case investigated in that study; very close source-term approximations are obtained when the exact mixture fraction PDF is used. Refer to project work done by Hickey *et al.* for further information on this issue. As Eq. 5.1 reveals there is a second component that determines the accuracy of the results: the chemistry table.

The way chemistry is implemented in CSE has turned out to suggest the method has an Achilles heel. When one inverts the integral equation for the conditional average of a species mass fraction, the result inevitably contains an error. When one does this for all of the species mass fractions in a particular mechanism (be they in an elementary kinetic mechanism or a skeletal or reduced one), the errors in the different species can end up being additive, such that elemental conservation is not ensured. In order to ensure elemental conservation, one would indeed have to invert for all species in the mechanism simultaneously subject to the constraints of both elemental conservation and positivity of all species mass fractions. While this is likely not impossible, it has never actually been tried, and clearly would be prohibitively expensive. As an alternative, we have been working with low dimensional manifold methods which pre-compute chemistry as a function of a dramatically reduced number of progress variables and store the result in a table. These have the advantage that not only are they dramatically less computationally expensive, but they also guarantee elemental conservation and positivity, provided one ensures that the progress variables used for the table lookup are actually contained in the table. For non-premixed the method of choice for reduced chemistry in previous research has been the Trajectory Generated Low-Dimensional Manifold (TGLDM) method.

3. Trajectory generated low-dimensional manifold

The first step in generating a TGLDM is to choose the progress variables that will be used. For non-premixed methane-air systems, mixture fraction and the mass fractions of the two main product species, CO_2 and H_2O have been used with much success [19, 22]. Next, a realizable composition space must be established. For methane-air combustion, Pope and Maas [28] proposed a realizable composition space based on the assumption that only major species are present on the boundary. The set of major species must be chosen by the user and for methane-air combustion may be taken as $\{\text{CO}_2, \text{H}_2\text{O}, \text{CH}_4, \text{O}_2, \text{CO}, \text{N}_2\}$ as suggested by Pope [29]. For a given mixture fraction Z , element conservation combined with the major species assumption can be used to generate the equations

$$f_{\text{H}/\text{CH}_4}Z = f_{\text{H}/\text{H}_2\text{O}}Y_{\text{H}_2\text{O}} + f_{\text{H}/\text{CH}_4}Y_{\text{CH}_4}$$

$$f_{\text{C}/\text{CH}_4}Z = f_{\text{C}/\text{CH}_4}Y_{\text{CH}_4} + f_{\text{C}/\text{CO}_2}Y_{\text{CO}_2} + f_{\text{C}/\text{CO}}Y_{\text{CO}}$$

$$f_{\text{O}/\text{Air}}(1 - Z) = f_{\text{O}/\text{O}_2}Y_{\text{O}_2} + f_{\text{O}/\text{CO}_2}Y_{\text{CO}_2} + f_{\text{O}/\text{CO}}Y_{\text{CO}} + f_{\text{O}/\text{H}_2\text{O}}Y_{\text{H}_2\text{O}}$$

Where $f_{j/i}$ is the mass fraction of element j in species i . Introducing the additional constraints $Y_{\text{CH}_4} \geq 0$, $Y_{\text{CO}} \geq 0$, $Y_{\text{O}_2} \geq 0$, $Y_{\text{CO}_2} \geq 0$ and rearranging the above equations leads to the following four inequalities that define the realizable region in CO_2 - H_2O space. The resulting boundary is shown in Fig. 2(a).

$$\begin{aligned}
Y_{CO_2} &\geq 0 \\
Y_{H_2O} &\leq \frac{f_{H/CH_4}}{f_{H/H_2O}} Z \\
Y_{H_2O} &\geq \frac{f_{H/CH_4} f_{C/CO_2}}{f_{H/H_2O} f_{C/CH_4}} Y_{CO_2} \\
Y_{H_2O} &\leq \frac{f_{O/Air}(1-Z) - (f_{O/CO_2} - \frac{f_{C/CO_2} f_{O/CO}}{f_{C/CO}}) Y_{CO_2}}{f_{O/H_2O} + \frac{f_{H/H_2O} f_{C/CH_4}}{f_{H/CH_4} f_{C/CO}} f_{O/CO}}
\end{aligned}$$

Trajectories are then generated by treating the chemistry as a homogeneous reactor, such that only the chemical reaction rates contribute to the change in the chemical state. Each trajectory is initialized at a discrete point along the boundary of the realizable composition space and the reaction rates are integrated until full chemical equilibrium is reached. The path taken through the composition space, when projected onto the lower dimensional surface described by the chosen progress variables is then the trajectory. Once the trajectories have been calculated, a common practice has been to represent them using Delaunay triangulation. This allows one to store the resulting manifold in a compact form from which lookup is relatively fast and simple; the table then contains all species mass fractions, temperature and chemical source-terms as a function of the progress variables (in the case of methane-air, mixture fraction and the mass fractions of CO_2 and H_2O), and, for any given combination of progress variables, one can look up the rates and mass fractions of all other species.

Unfortunately, even for methane-air combustion at moderate pressures, trajectories will often cross one another, which significantly complicates the triangulation. What has been done in the past is to decide on a "fundamental" trajectory, which dominates all others – this is usually chosen to be the one beginning at the origin – and then any trajectory that crosses this trajectory is truncated at the crossing point. For methane-air systems, a typical manifold prior to trajectory truncation is shown in Fig. 2(b).

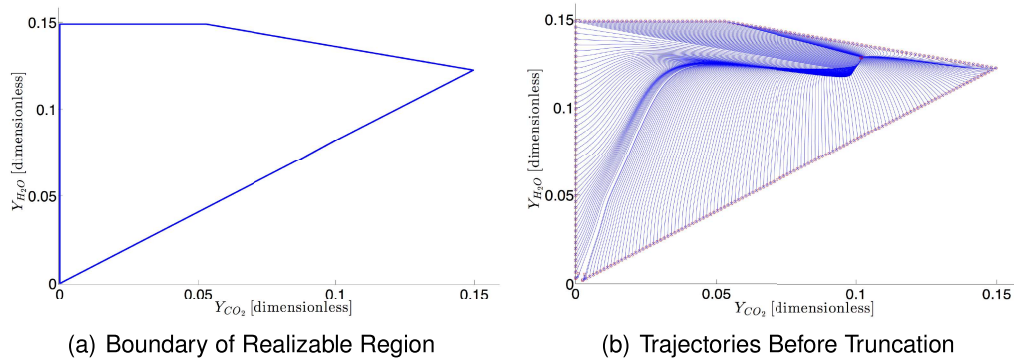


FIGURE 2. CH_4 -Air Manifold Using Major Species Assumption, $Z = 0.0663$, $P = 1$ atm

For methane-oxygen at high pressure, not only do many more trajectories cross than did for methane-air, a new problem arises: trajectories appear to leave the realizable composition space. Indeed, for some mixture fractions, the equilibrium point is outside

of the realizable composition space as shown in Fig. 3. It should be noted that this does not represent an unphysical composition of the mixture, but rather is a consequence of the arbitrary nature of the major species selection. To correct this, the definition of the realizable composition space has been re-examined.

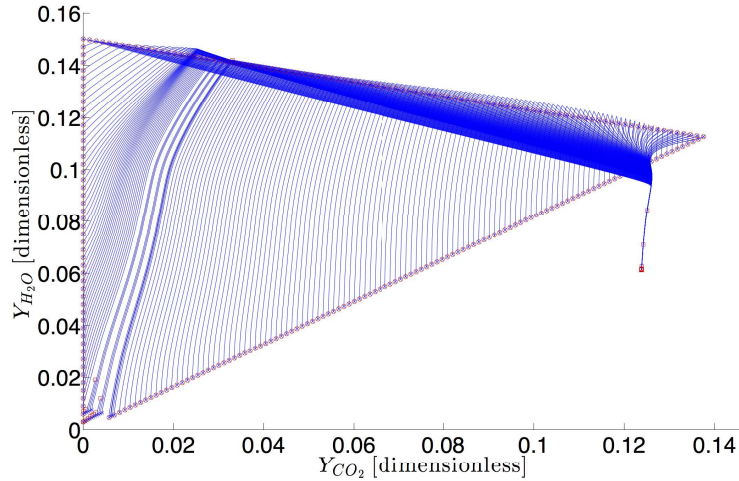


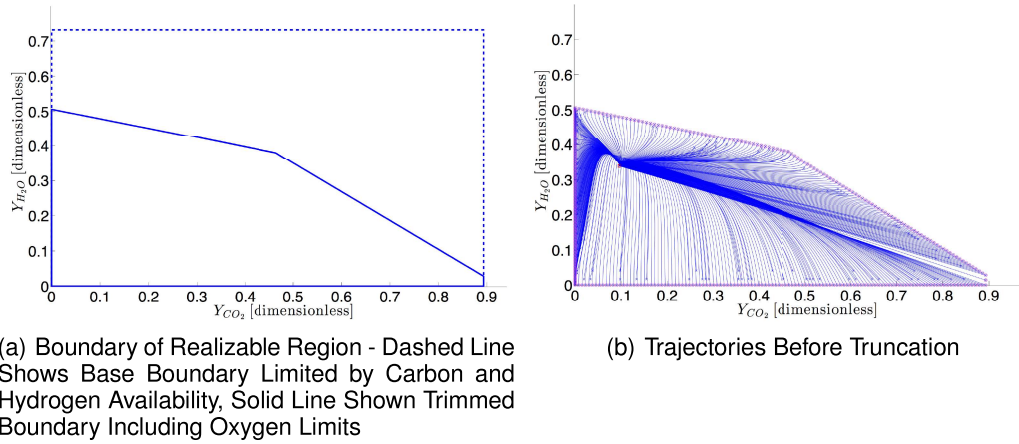
FIGURE 3. $\text{CH}_4\text{-O}_2$ Manifold Using Major Species Assumption, $Z = 0.8$, $P = 20$ bar

A new realizable composition space has been created by expanding the region so that the maximum CO_2 and H_2O mass fractions are defined by the total amount of carbon and hydrogen atoms present at the given mixture fraction, respectively. This creates a rectangular boundary which is the base for the new realizable region. For each point on this boundary the remaining elements are placed into a minimum number of additional species which are chosen so as to allow for only one possible composition while conserving elements. For example, on the left hand boundary in Fig. 4(a) there is no CO_2 present, and the H_2O mass fraction is constrained. The additional species are therefore chosen as CH_4 , CO , and O_2 as this ensures that there is only one possible combination of these species that conserves elements. At higher mixture fractions, there is not enough oxygen to reach one or both of the upper corners of the rectangle without generating negative species concentrations, and thus the boundary is modified by clipping these regions as shown in Fig. 4(b).

The new expanded boundary ensures that the equilibrium point remains inside the realizable region for all mixture fractions, however it does not address the issue of crossing trajectories. Nonetheless, using the new realizable region and truncating those trajectories that cross the fundamental trajectory has allowed for a high pressure Methane-Oxygen TGLDM table to be constructed and tested in the simulation.

4. Simulation

The objective for the summer program had been to evaluate the applicability of CSE as a model for the turbulence-chemistry-interaction in high-pressure combustion. This project was linked to the project by Hickey *et al.* on the development of an improved PDF model for high-pressure combustion to conduct a RANS simulation under similar conditions with $\text{CH}_4\text{-O}_2$ -combustion present. The test case chosen for this study is a

FIGURE 4. CH_4 -Air Manifold Using Expanded Realizable Region, $Z = 0.32553$, $P = 20$ bar

single-injector of methane- O_2 -combustion, which was carried out for the last summer program and has been simulated by multiple groups in the past - allowing for a comparison to e.g. the flamelet computations carried out by the DLR with the TAU code solver.

Due to the limited time frame of the summer program, a RANS simulation was proposed. However, LES would be the preferred long-term approach to account for the complexities associated with the small-scale physics.

Major issues associated with the initialization and the chemistry prevented a successful simulation of the test case and therefore no comparison could be made. However the findings of the project significantly contribute to the understanding and allow for a detailed analysis and evaluation of the applicability of the CSE method under the given conditions. The complementary project by Hickey *et al.* revealed more insight into the correlation of thermodynamic properties in high-pressure combustion and its effect on the combustion progress.

4.1. Initialization

The combustion chamber is 300 *mm* long and has an inner square cross section of 12 *mm* \times 12 *mm*.

Methane is injected with a co-axial injector at 0.017 *kg/s* and oxygen at 0.045 *kg/s*. A detailed schematic of the experimental setup is presented in Fig. 5(a) and the mesh generated for the numerical simulation using RANS in Fig. 5(b).

For initialization a variety of options are available and listed in Tab. 1.

In all cases of potential initialization combinations, that were tested, it seemed necessary to have a developed velocity field in the domain of the internal field in order to avoid sudden jumps in thermo-physical properties. When initializing with pure methane or oxygen content, a kind of autoignition occurs causing high chemical source terms. With a high mass fraction in the products CO_2 and H_2O the chemical and enthalpy source terms are highly negative as the composition evolves to equilibrium. That causes strong fluctuations in temperature within the combustible region of the domain. First encounters with this problem lead the investigation to a detailed review of the chemistry table generated using the TGLDM method and the method itself. The results of this investigation are provided in section 4.2.

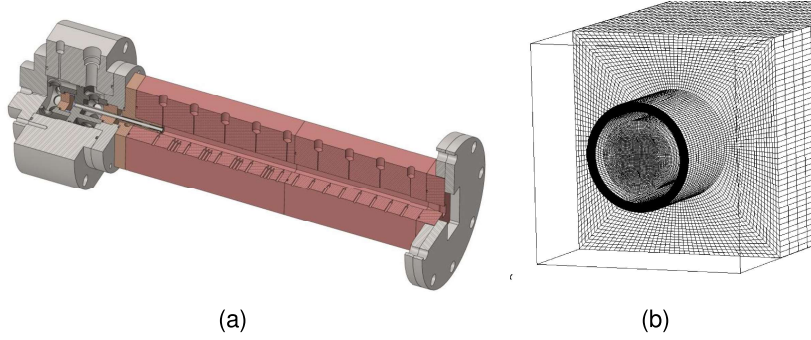


FIGURE 5. (a) Experimental setup and (b) mesh for single injector test case

TABLE 1. Categorization of the initialization options at hand

Attribute	Option		
	1	2	3
Initial field	CH ₄ flush	O ₂ flush	Stoichiometric equilibrium composition
Temperature	cold	cold	hot
Ignition	autoignition ignition kernel hot spot on wall	autoignition ignition kernel hot spot on wall	autoignition
Regularization	Previous time step Laminar Flame Solution	Previous time step Laminar Flame Solution	Previous time step

Efforts directed towards controlled temperature increase using a hot spot or an ignition kernel at combustion initialization resulted in a delay of the temperature fluctuation effects, but nonetheless appeared in the same manner eventually.

The regularization of the inversion in CSE provides a major knob for steering the initialization of the simulation. Regularizing to a laminar flame solution allows for more control on the stability, but the source terms are being extracted from the same chemistry table and therefore the temperature fluctuations remain.

4.2. Chemistry

Despite the fact that a fully defined manifold is available for the CH₄-O₂ combustion, additional issues arose during simulation. A detailed investigation on the manifold revealed that certain compositions temperatures of unphysical nature were present in order to maintain constant enthalpy throughout the realizable space. Fig. 6(a) shows location of these compositions in and around the upper right-hand corner of the manifold at stoichiometric conditions. The same phenomena is present for a variety of mixture fractions within the flammability limits. A comparison with the manifold in Fig. 6(b), that would be available for CH₄-Air combustion under high pressure conditions, shows that

the extreme temperatures in the manifold result from the use of oxygen as an oxidizer rather than air and not from the high pressure conditions.

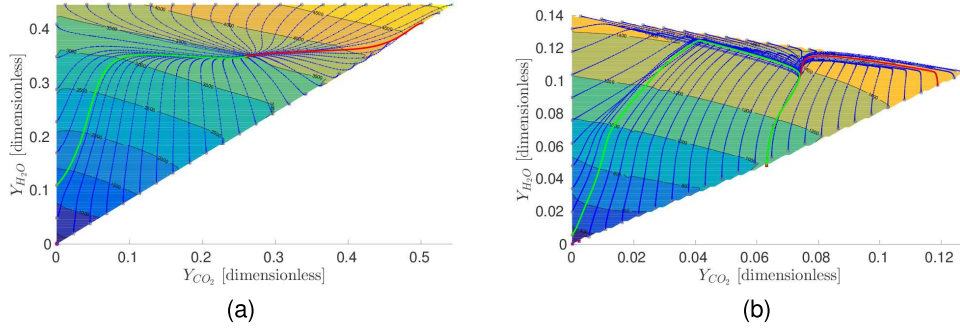


FIGURE 6. Temperature distribution in manifold for (a) $\text{CH}_4\text{-O}_2$ (b) $\text{CH}_4\text{-Air}$ combustion under high pressure conditions

As the trajectories evolve from their starting point on the boundary of the realizable region the calculation of all source terms and all thermodynamic properties is dependent on the temperature of the starting point and its evolution. The unphysical nature of some of these points has an effect on the chemical source term, but also on the enthalpy source term, which is included in the resulting chemistry table. Two trajectories each were selected from the manifolds in Fig. 6 to examine the source terms. A comparison between the oxygen based and the air based minimum and max values shows, that the oxygen based manifold contains some extremely low enthalpy source terms, which would explain the sudden drops in temperature in the simulation in regions of high H_2O concentration. Trajectory A (green) in Fig. 7(a) and 7(b) shows a significant positive enthalpy source term on the path towards equilibrium with a very reasonable order of magnitude. However trajectory B (red) takes on extremely low values in Fig. 7(a) compared to the maximum value of trajectory A and it is seven orders of magnitude greater than the minimum value in methane-air combustion case. The same trends can be followed in Fig. 7(c) and 7(d). As the temperature greatly effects the reaction rates, it is to be expected that those too are of unphysical nature in the equivalent regions of the manifold.

In light of this discovery an attempt was made to clip the manifold based on (a) temperatures 10% above the equilibrium temperature (b) temperatures above a threshold of 3800 K and (c) a threshold of -10^{10} for the enthalpy source term.

(a) Too radical in that the residual manifold does not provide a way to significantly reduce the CO_2 and H_2O mass fractions as those regions of the manifold are cut off.

(b) Temperature fluctuations remain an issue, but mass fractions stay within reasonable range.

(c) Temperature fluctuations remain an issue and depending on the initialization options the mass fractions tend to go out of range as well.

These findings lead to the conclusion of a strong dependency of the system on the temperature and other thermo-physical properties making the TGLDM method in its current state unsuitable for $\text{CH}_4\text{-O}_2$ combustion simulation in combination with traditional CSE. It must be noted that this conclusion is highly in line with results of the other CSE-related project by Hickey *et al.*, in which the PDF modeling was the focal point and revealed a strong dependency of the accuracy of the chemistry source term with

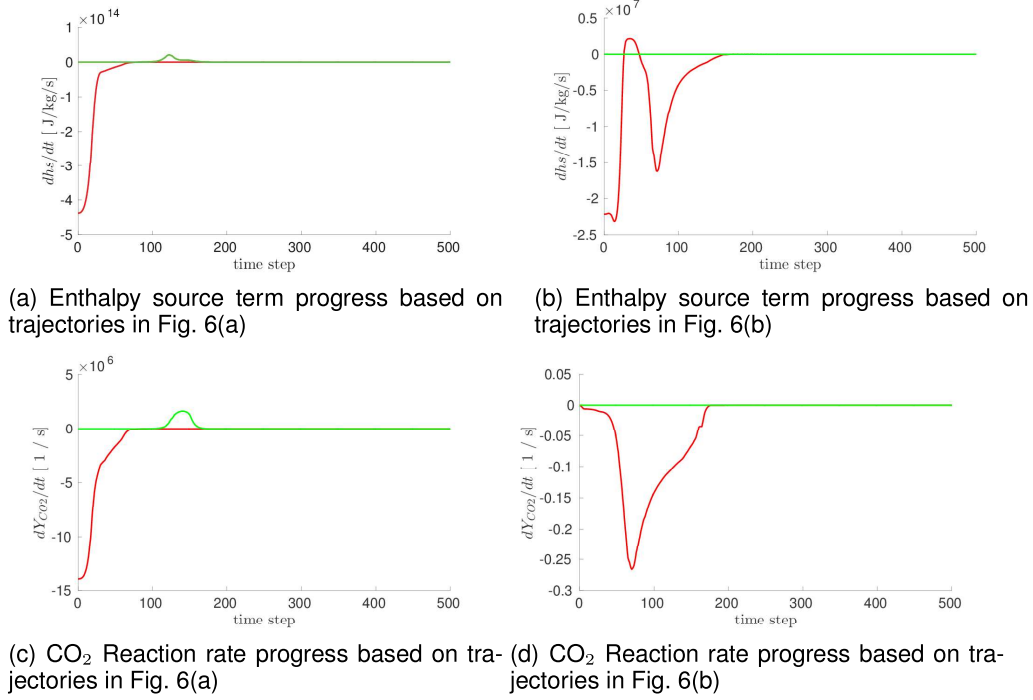


FIGURE 7. Source term progress along trajectories as per indication in the manifold in Fig. 6, where the green line and the red line correspond to the trajectory originating in the bottom left-hand corner of the manifold and the top right-hand corner of the manifold respectively

the temperature as a second conditioning variable besides the commonly used mixture fraction. It suggests that it might be necessary to use a second condition, as is done in DCSE, however this would also have implications for how one creates the manifold, as it would clearly be necessary to include temperature as a dimension somehow and it is not obvious how this could be done within the current TGLDM framework. It is hoped that this will be pursued in future work.

5. Conclusion

This project lent itself to an investigation of the applicability of Conditional Source-term Estimation (CSE) in high-pressure CH₄-O₂ combustion as well as an evaluation on the reduced chemistry method TGLDM, which commonly used in non-premixed combustion. The essence of CSE is the utilization of a conditioning variable – here mixture fraction – to account for the turbulence-chemistry interaction via the following equation:

$$\bar{\omega}_k = \int_0^1 \left(\bar{\omega}_k | \zeta \right) P(\zeta) d\zeta. \quad (5.1)$$

The accuracy of the model therefore depends on the conditional source term, which is given by the reduced chemistry table, and on the PDF model. This project revealed that the TGLDM method in it's current state is not suitable for CH₄-O₂ combustion due to it's underlying assumptions on the constant enthalpy within a manifold. Applying this constraint leads to regions of unphysical temperature, which in turn affect the chemical

source terms. In the simulation a strong temperature dependency is evident and so it can be concluded that the TGLDM method in combination with the traditional CSE approach is not applicable to high-pressure $\text{CH}_4\text{-O}_2$ combustion.

Taking into consideration the findings from the collaborative project by Hickey *et al.* provides further validation for the latter statement. The work on modeling the probability density function (PDF) of the mixture fraction for high-pressure turbulent combustion showed that conditioning on the mixture fraction alone is insufficient to characterize the chemical source term. While conditioning on mixture fraction with CSE provides a good means to account for turbulence-chemistry interaction, the thermodynamic effects present in high-pressure combustion have a significant impact on this interaction as well. In order to account for the chemistry-thermodynamic interaction a second conditioning variable is necessary and therefore a DCSE method is required to overcome the challenges at hand. Furthermore the investigation showed, that temperature would be a prime candidate for the choice of a second conditioning variable to achieve significant improvement in the modeling of the PDF and with that the accuracy of the CSE method.

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